



Crossbar Architecture for Molecular Electronics

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Abstract

Although most of the applications of molecular electronics are far away from us, people still have confidence in molecular electronics. So far, researchers have discovered a series of electrical, optical, and optical chirality properties of various molecules for replacing the existing electronic components with the new features. However, there are still many challenges on the way to make molecular circuits and even assemble molecular computers. In this poster, we describe an idea that uses molecular properties and crossbar architecture to build a reprogrammable memory/logic circuit.

Introduction

In the late 1950s, “Molecular electronics” was firstly proposed. In 1959, Richard Feynman gave a speech “There’s Plenty of Room at the Bottom” at the California Institute of Technology. Based on nanotechnology, people have more thoughts about the micro world. In 1974, Arieh Aviram and Mark Ratner published “Molecular Rectifiers”. This paper is regarded as the pioneering work of molecular electronics. The idea of molecules as electronic components is extremely revolutionary and subversive at that time. In the last 30 years of the last century, the concept of molecular computers has gradually formed, and molecular electronics has also become a subject.

Therefore, what is exactly “molecular electronics”? From above, the idea of molecular electronics was initially to use molecules as electronic components, so that the size of electronic components at that time would be greatly reduced. So far, researchers have discovered a series of electrical, optical, and optical chirality properties of various molecules for replacing the existing electronic components with the new features. However, there are still many challenges on the way to make molecular circuits and even assemble molecular computers.

The cornerstones of molecular electronics are traditional disciplines, physics, chemistry, materials science, electronic engineering and biology. It is necessary to analyze phenomena with quantum theory, and to study electronic behavior and thermodynamics at the molecular level. Thus, it is also considered as a branch of nanoelectronics. From a technical point of view, the main advantages of molecular electronics have been proposed at early stage: size, speed, cost, and new characteristics. Currently, molecules are used in the research of electronic components: molecular transistor, molecular switch, molecular wires, molecular capacitance, molecular insulators, etc. Crossbar architecture is similar to the array architecture of memory, hence it offers the advantage of fault tolerance and redundancy repair. Molecular electronics is fabricated with bottom-up self-assembly, which generally lead to high defect density. If any molecular switch is faulty, it can be easily switched off and replaced with a redundant row and column. This is essential to ensure the molecular memory/circuit can work properly even with the defects in the molecular switches.

In this poster, we selected a molecule that has been modified to be used as a light-driven molecular electronic switch. By using this molecule, it is possible to design a circuit with a crossbar structure. The circuit has two modes that can be either used for a memory device or a logic device, such as decoder or full adder.

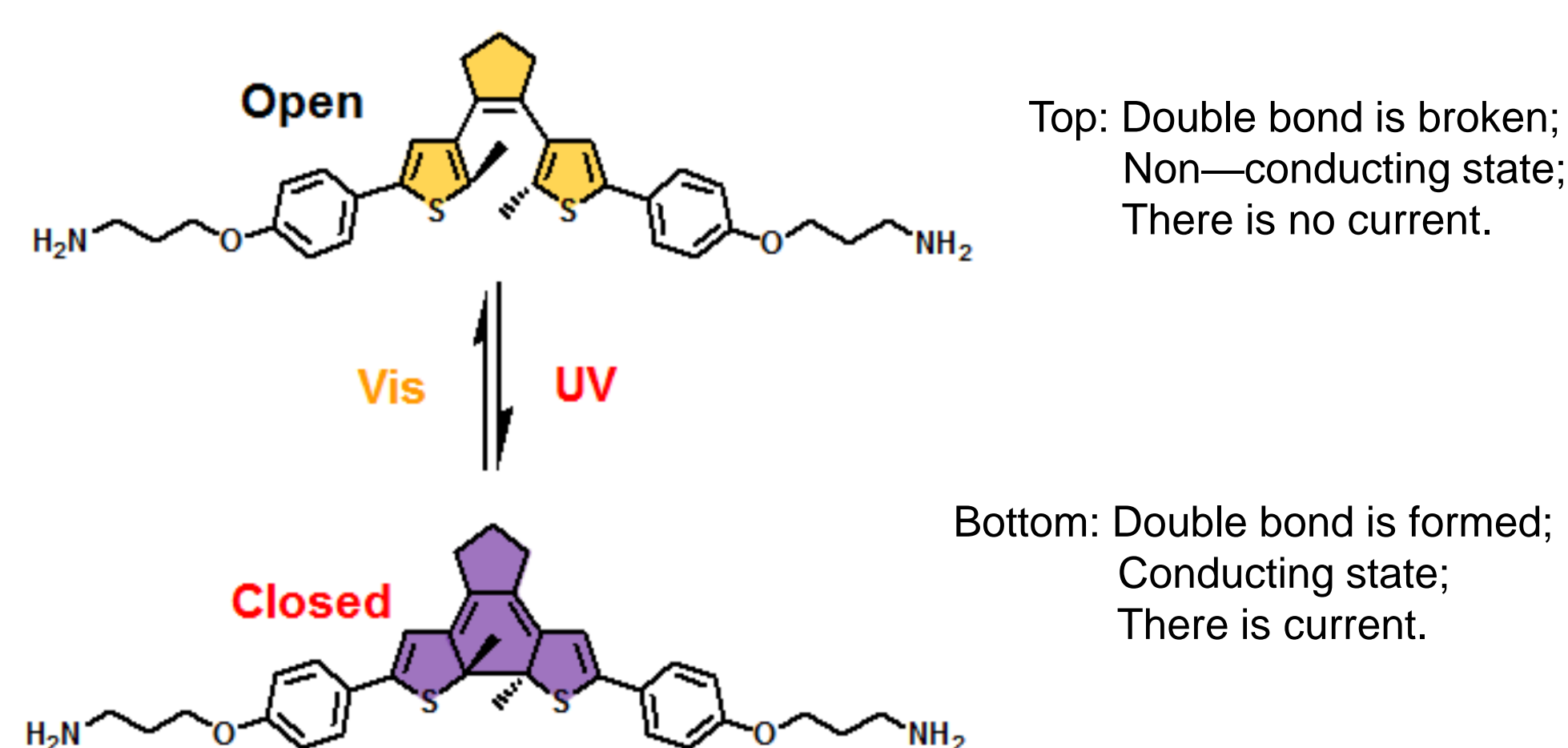


Figure 1. **Diarylethene** - schematic of the transitions between the open and closed molecular conformations under UV and visible irradiation (Jia, C. et al., 2016))

Diarylethene for molecular electronics

Figure. 1 shows a modified diarylethylene for a reversible electrical conduction light-driven molecular switch. Jia, C. et al. (2016) merged three methylene (CH₂) groups on each end of the diarylethylene molecular backbone. As a result, the molecule becomes conductive under visible irradiation; while it becomes non-conductive under ultraviolet irradiation. Its *I/V* characteristics is described in figure 2.

To realize the practical application of molecular electronics, the first task is to face three problems in turn: 1). What are the characteristics of the molecule as a molecular electronic component? 2). Fabrication: how the molecular unit (single molecule, or cluster, or a layer) will be assembled into the circuit? 3). Logic circuit assembly. A modified diarylethylene proves itself as a molecular switch. For solving the second question, “crossbar” structure is one efficient option that can be fabricated by nanoimprint lithography. Similar to a “sandwich”, the bottom and top are nano metal electrode layers, and one molecular film layer is placed in the middle. Both ends of the molecule can be chemically modified so that one end is hydrophilic and the other end is hydrophobic. Amphoteric molecules can be transported and assembled between two metal layers through a solid film. In next section, it mainly explains the assumptions about the function and logic.

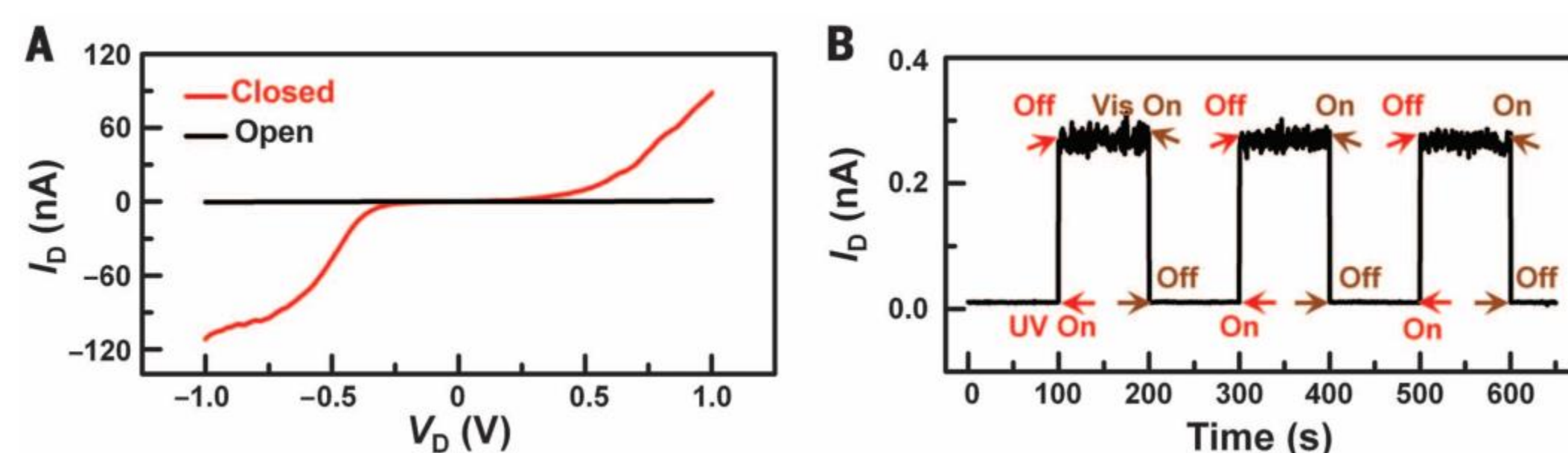


Figure 2. (A) *I-V* characteristics of individual diarylethenes in open (black line) and closed (red line) form at gate voltage $V_G = 0$ V. V_D , drain voltage; I_D , drain current. (B) Real-time measurement of the current through a diarylethene molecule that reversibly switches between the closed and open forms, upon exposure to ultraviolet (UV) and visible (Vis) radiation, respectively. $V_D = 100$ mV and $V_G = 0$ V. (Jia, C. et al., 2016))

Crossbar molecular circuit

1). Memory mode

The proposed crossbar molecular circuit have two modes: memory and logic mode. Figure 3. shows the schematics of the memory. Independent light-path tunnel should be fabricated for each cell, so that each cell can be written as either “0” (Open) or “1” (Closed). Orange wires are the top electrodes layer. Red and green solid dots are diarylethylene molecular layer. Purple wires are connectors in between. Black wires are the top electrodes layer. “Write” and “Erase” operations are manipulated through Vis and UV lights. “Read” through two-dimensional addressing.

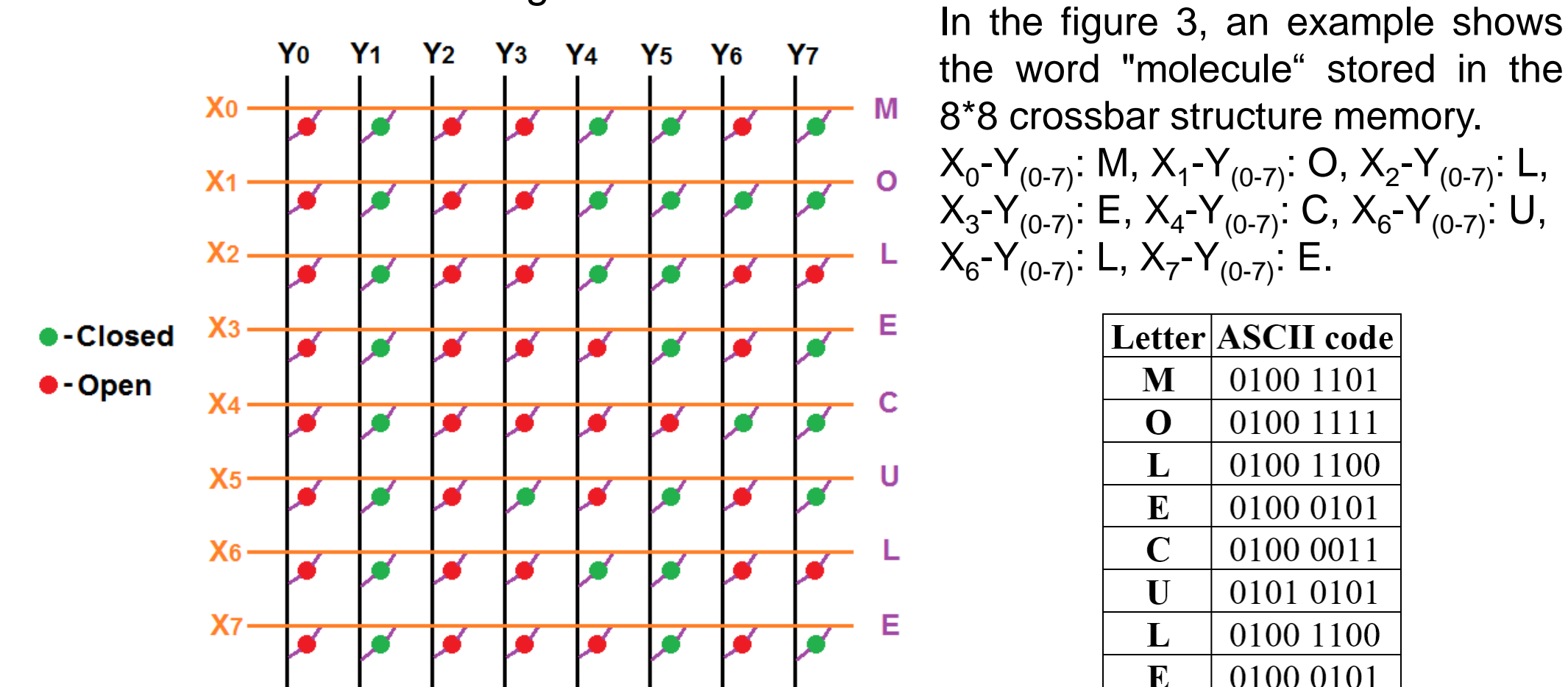


Figure 3. The crossbar memory configuration for storing the word “MOLECULE”

2). Logic mode

The proposed device can be switched to a combinational logic device by pre-setting the value in each cell. Figure 4. shows a example of building a 3-bit decoder. A, B, C (bottom layers) are inputs. By reading the threshold (three pathways) current from $X_{(0-7)}$, the output shows as they are in table 1. Once the 3-bit decoder is achieved, a full adder, as in figure 5, can be built based on the decoder and its neighboring memory. $X_{(0-7)}$ wires are used as selection wires according to the decoder; while, $X_{(0-7)}-Y_6$ and $X_{(0-7)}-Y_7$ are a memory module for storing output values. For example, if $A = 1$, $B = 0$, and C (C_{in}) = 1, the X_5 will be selected, and the values at X_5-Y_6 and X_5-Y_7 will be read as $C_o = 1$, Sum = 0.

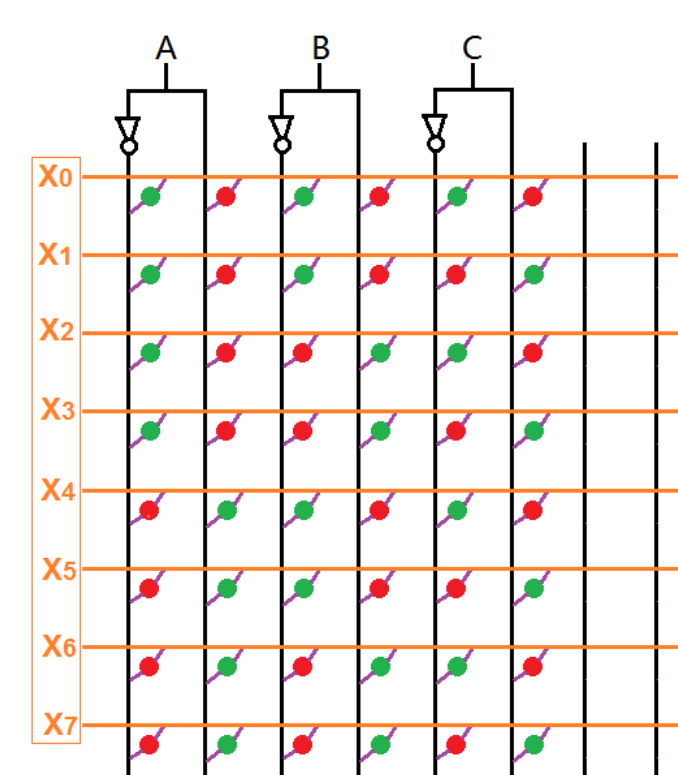


Figure 4. 3-bit decoder

Table 1. Truth table of the 3-bit decoder

#	ABC	X ₀	X ₁	X ₂	X ₃	X ₄	X ₅	X ₆	X ₇
0	000	1	0	0	0	0	0	0	0
1	001	0	1	0	0	0	0	0	0
2	010	0	0	1	0	0	0	0	0
3	011	0	0	0	1	0	0	0	0
4	100	0	0	0	0	1	0	0	0
5	101	0	0	0	0	0	1	0	0
6	110	0	0	0	0	0	0	1	0
7	111	0	0	0	0	0	0	0	1

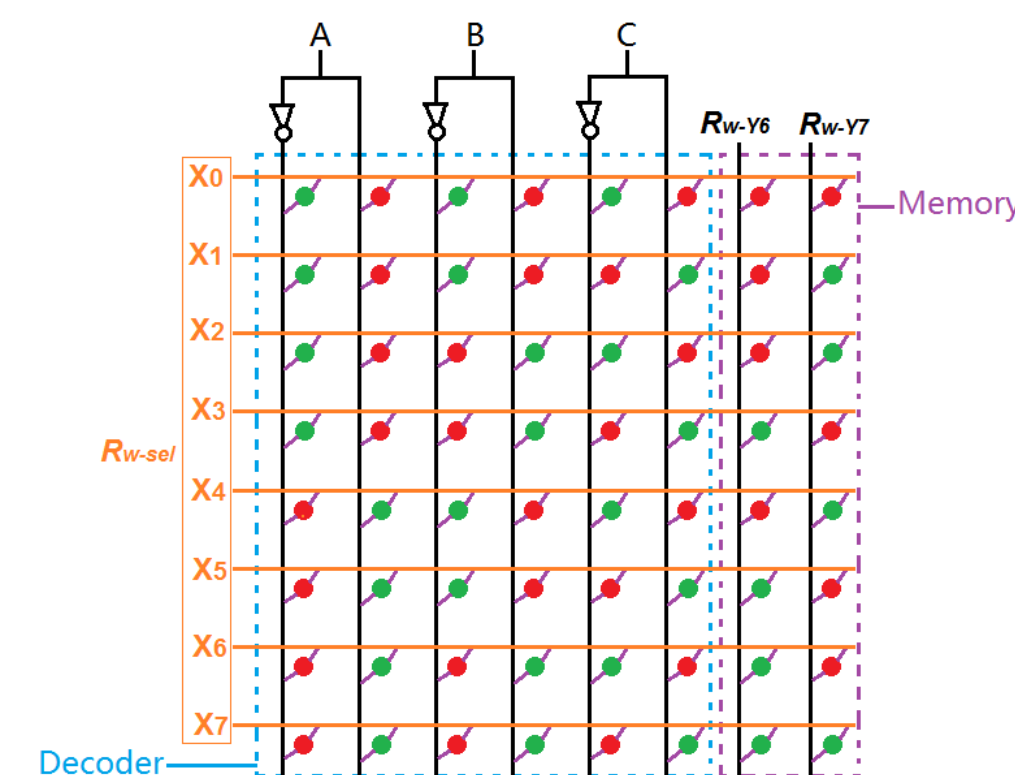


Figure 5. 1-bit full adder

Table 2. Truth table of the 1-bit full adder

#	ABC	(Co) Y ₆	(Sum) Y ₇
0	000	0	0
1	001	0	1
2	010	0	1
3	011	1	0
4	100	0	1
5	101	1	0
6	110	1	0
7	111	1	1

Conclusion

The design above is mainly about how to use molecular switches to build reprogrammable mem/logic circuit units. The scheme is still very immature, and there are many potential problems that need to be solved in the following work. For example, the applied molecular switch is a bidirectional conductive switch, and the circuit itself lacks rectifying components. With the crossbar structure, the “snake current” is inevitable, and it is a big problem. It is also necessary to further study the resistance characteristics of the molecules. The expansion of the system will result in more complicated operations of voltage/current.

References

- [1] Jia, C.,et al. (2016). Covalently bonded single-molecule junctions with stable and reversible photoswitched conductivity. *Science*, 352(6292), 1443–1445. doi:10.1126/science.aaf6298
- [2] Wu, W., et al. (2005). One-kilobit cross-bar molecular memory circuits at 30-nm half-pitch fabricated by nanoimprint lithography. *Applied Physics A*, 80(6), 1173–1178.
- [3] Zhong, Z., et al. (2003). Nanowire Crossbar Arrays as Address Decoders for Integrated Nanosystems. *Science*, 302(5649), 1377–1379. doi:10.1126/science.1090899